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Mixing Martini: Electrostatic Coupling in Hybrid Atomistic – Coarse-Grained Biomolecular Simulations

Tsjerk A. Wassenaar^{§,§}, Helgi I. Ingólfsson^{§,§}, Marten Prieß[#], Siewert J. Marrink[§], and Lars V. Schäfer^{#,}*

[§]Groningen Biomolecular Sciences and Biotechnology Institute & Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 7, 9747 AG Groningen, The Netherlands

[#]Institute of Physical and Theoretical Chemistry, Goethe University Frankfurt, Max-von-Laue-Str. 7, D-60438 Frankfurt am Main, Germany

*email: schaefer@chemie.uni-frankfurt.de

[§] These authors contributed equally to this work.

Table S1. Maxima and minima of the PMFs. Local maxima and minima are given in *italic*.

	d (nm)	ΔG (kJ/mol)	d (nm)	ΔG (kJ/mol)
Na⁺/Cl⁻				
SPC/E	0.25	-8.2	0.35	5.3
PW (CG)	0.46	-9.1	0.67	0.1
BMW (CG)	0.46	-9.5	2.11	0.1
NaCl(0) PW	0.31	-6.2	0.66	3.1
PW 1.0	0.23	193.3	0.36	227.5
PW 1.1	0.23	83.0	0.41	147.4
PW 1.25	0.23	-33.6	0.47	73.9
PW 1.3	0.24	-57.4	0.48	57.7
PW 1.45	0.23	-137.3	0.56	21.5
PW 1.5	0.23	-155.4	0.57	13.5
PW 2	0.26	-271.6		
BMW 1.0	0.23	-93.2	0.50	38.9
BMW 1.1	0.23	-150.3	0.56	14.3
BMW 1.2	0.23	-195.9	2.16	0.0
BMW 1.3	0.23	-231.8	2.04	0.1
BMW PME	0.46	-7.9	0.65	0.8
PW PME	0.46	-7.2	0.67	1.9
Lys/Glu				
SPC/E	0.53	-3.2	0.65	-2.8
	0.92	-3.3	2.05	0.0
PW (CG)	0.46	-5.2	0.75	-0.7
	0.94	-2.7	2.08	0.1
BMW (CG)	0.46	-2.7	0.71	-1.7
	0.92	-4.2	2.05	-0.1
Std CG water $\epsilon=15$	0.47	-11.0	2.12	0.1
Std CG water $\epsilon=78$	0.50	-2.6	0.76	1.4
PW $\epsilon=1.0$	1.34	-7.8		
PW $\epsilon=1.45$	0.44	-8.7	0.65	5.0
PW $\epsilon=1.5$	0.44	-20.7		
BMW $\epsilon=1.0$	1.00	-1.4	1.15	-0.8
	1.40	-1.8	1.99	0.3
BMW $\epsilon=1.1$	0.46	-8.7	0.66	4.8
BMW $\epsilon=1.15$	0.46	-30.6	0.71	0.2
BDW $\epsilon=2.3$	0.49	-156.2		
Glu/Glu				
SPC/E 2Na ⁺	0.64	3.2	0.74	3.7
	0.91	2.7	0.97	2.7
	2.03	-0.1	2.16	0.0
SPC/E no counterions	0.65	5.5	0.73	5.7
	0.92	4.5	0.94	4.5
PW (CG)	1.80	-0.2	2.08	0.0
BMW (CG)	0.91	2.9	1.06	3.5
PW $\epsilon=1.45$ 2Na ⁺	0.51	-3.9	0.65	-1.6
	0.79	-4.3	1.09	3.4
PW $\epsilon=1.45$ no counterions	0.50	0.7	0.70	4.9
	0.82	3.9	1.09	6.2
PW $\epsilon=1.75$ 2Na ⁺	1.82	0.2	1.96	0.4
BMW 1.1 2Na ⁺	0.80	-3.5	1.08	2.8
BMW 1.1 no counterions	0.80	-0.9	1.06	4.6
Ser/Ser				
SPC/E	0.44	-1.0	0.61	0.8
PW (CG)	0.52	-2.0	0.73	2.2
BMW (CG)	0.94	-1.7	1.21	1.2

Std CG water	0.33	-22.2	0.69	2.6
PW $\epsilon=1.0$	0.32	-20.4	0.67	3.3
PW $\epsilon=1.45$	0.33	-20.3	0.68	2.8
PW/s $\epsilon=1.45$	0.33	-16.0	0.61	1.8
BMW $\epsilon=1.1$	0.32	-15.3	0.59	4.9
BMW/s $\epsilon=1.1$	0.33	-10.2	0.54	3.2
BDW $\epsilon=2.3$	0.33	-3.8	0.41	0.9

NMA/NMA

SPC/E	0.45	-3.0	1.95	0.0
Std CG water	0.45	-20.3	1.17	0.3
PW $\epsilon=1.0$	0.38	-9.4	0.68	0.2
PW $\epsilon=1.45$	0.44	-10.9	0.74	1.2
BMW $\epsilon=1.1$	0.44	-6.7	1.75	0.4
BDW $\epsilon=2.3$	0.46	-3.5	1.57	0.1

Phe/Phe

SPC/E	0.53	-2.8	0.82	0.4
PW (CG)	0.57	-6.4	0.90	1.6
BMW (CG)	0.68	-2.0	0.82	-0.5
	1.03	-2.6	1.36	0.6
Std CG water	0.51	-4.3	0.85	2.2
PW $\epsilon=1.45$	0.52	-3.6	0.85	2.0
BMW $\epsilon=1.0$	0.65	2.3	0.75	2.6
	1.03	-1.3	1.32	1.5
BMW $\epsilon=1.1$	0.63	2.7	0.74	3.0
	1.04	-1.4	1.34	1.4
BDW $\epsilon=2.3$	0.56	-1.7	0.85	0.3

Val/Val

SPC/E	0.49	-2.0	0.68	1.0
PW (CG)	0.51	-5.5	1.17	0.4
BMW (CG)	0.55	1.0	0.65	2.2
	0.91	-0.5	1.19	1.9
PW	0.45	-6.0	0.76	0.6
BMW	0.46	-0.7	0.66	1.5
	0.92	-1.5	1.21	1.0
Std CG water	0.45	-6.5	1.18	0.3
BDW	0.52	-2.1	0.79	0.8